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# Cluster development of the density matrices in the Jastrow method for many-fermion systems

By S. O. Lundqvist

ABSTRACT

A method is given for the cluster development of the reduced density matrices for Jastrow wave functions. The essence of the method is to make extensive use of the simple properties of the Dirac density matrices corresponding to the uncorrelated motion, in conjunction with the method of expanding the distribution functions for a classical imperfect gas given by Mayer and Montroll.

## Introduction

In the original paper by Jastrow [1], he discusses the case of a uniform Fermi gas. Starting from the cluster expansion of the pair distribution function for a classical gas and taking the antisymmetry requirement into account in an approximate way, he derived an approximate expression for the energy of the gas. A more general derivation, not restricted to uniform systems and taking account of the exclusion principle, was later given by Iwamoto and Yamada [2], who made use of a transformation introduced by Ursell [3] in the theory of imperfect gases. They only consider the cluster development of the energy so no information about the distribution functions is obtained from their work. Recently a detailed discussion has been given by Hartogh and Tolhoek [4] of the distribution functions for a uniform Fermi gas, neglecting spin.

In the present note a different method will be indicated, which is not restricted to a uniform gas and in which spin and isobaric spin is taken into account from the beginning. The method has some similarity to that used by Hartogh and Tolhoek, but differs from theirs by making extensive use of the simple properties of the Dirac density matrices for the system [5]. No special attention has to be given to the fulfilment of, e.g., conservation of linear or angular momentum components, because such conservation principles are already contained in the Dirac matrices, if the one-particle functions are properly chosen.

## The reduced density matrices for Jastrow wave functions

We consider a system of $A$ fermions with equal masses $m$, which interact with two-body forces described by a potential $v = v(i,j)$, where i and $j$ stand for the coordinates (including spin and isospin) of the particles $i$ and $j$. Let us introduce the reduced density matrix for $n$ particles [6]

$$(1'2' \dots n' | \varrho | 1 2 \dots n) = \\ = \frac{A!}{(A-n)!} \frac{\int \Psi^* (1'2' \dots n', n+1 \dots A) \Psi (1 \dots n, n+1 \dots A) \, d\tau^{A-n}}{\int \Psi^* (1 \dots A) \Psi (1 \dots A) \, d\tau^A} \tag{1}$$

where $\psi(1 \dots A)$ is the wave function for the system. $d\tau$ implies summation over discrete as well as integration over continuous variables. The normalization of (1) is chosen such that the diagonal element represents the probability density for $n$ particles. The expectation value of the energy can be expressed by means of the reduced density matrices for one and two particles as follows:

$$E = \frac{1}{2m} \int d\tau_1 (1 | p_1^2 \varrho | 1) + \frac{1}{2} \int d\tau_1 d\tau_2 (1 2 | v \varrho | 1 2). \tag{2}$$

Here $p_1$ denotes the momentum operator of particle one and the symbols $(1 | p_1^2 \varrho | 1)$ and $(1 2 | v \varrho | 1 2)$ mean ordinary matrix products.

As a trial function for the ground state of the system we write

$$\psi(1 \dots A) = F \, \Phi(1 \dots A), \tag{3}$$

where $\Phi(1 \dots A)$ describes the uncorrelated motion and is taken as a Slater determinant of suitably chosen one-particle functions $\varphi_\nu(i)$, and $F$ is an operator describing the correlations.

In the Jastrow method one chooses

$$F = \prod_{i<j} f(ij), \tag{4}$$

where the two-particle correlation function $f(ij)$ satisfies the symmetry condition

$$f(ij) = f(ji) \tag{5}$$

and the boundary condition

$$f(ij) \to 1, \qquad r_{ij} \to \infty. \tag{6}$$

We shall restrict ourselves to the case where $f(ij)$ depends only on the position and spin and isospin of the particles. It would be desirable to include also a dependence on the states of the particles $i$ and $j$. In such a case (4) has to be replaced by the symmetrised product of the $f(ij)$. This more general case can easily be treated by an extension of the method used here.

In the following we shall make use also of the density matrices, corresponding to the uncorrelated motion [5]

$$\langle 1' \dots n' | \varrho | \dots n \rangle = \\ = \frac{A!}{(A-n)!} \int \Phi^* (1' \dots n', n+1 \dots A) \Phi (1 \dots n + n + 1 \dots A) \, d\tau^{A-n} \tag{7}$$

if $\Phi$ is normalized to unity.

These matrices for all $n$ are determined by the one-particle density matrix

$$\langle i'|\varrho|i\rangle = \sum_{\nu} \varphi_{\nu}^{*}(i')\,\varphi_{\nu}(i) \tag{8}$$

according to

$$\langle 1' \dots n'|\varrho|1 \dots n\rangle = \det_n\{\langle i'|\varrho|i\rangle\}. \tag{9}$$

Using (3), (4) and (7) we can write (1) in the form

$$(1' \dots n'|\varrho|1 \dots n) = \\ = \frac{A!}{(A-n)!}\,\frac{\int F^{*} F \langle 1' \dots n', n+1 \dots A|\varrho|1 \dots n, n+1\rangle\, d\tau^{A-n}}{\int F^{*} F \langle 1 \dots A|\varrho|1 \dots A\rangle\, d\tau^{A}}. \tag{10}$$

## Cluster development of the $n$-particle density matrix

The expansion of $(1' \dots n'|\varrho|1 \dots n)$ can be performed by a simple extension of the method introduced by Mayer and Montroll [7] for an imperfect classical gas. It is convenient to introduce the notation

$$Q(A-l) = \prod_{j>i>l} g(ij), \tag{11}$$

where

$$g(ij) = f^{*}(ij)\,f(ij) = h(ij) + 1. \tag{11'}$$

To simplify the notation the primes on certain quantities will not be written out in the following. For instance, if $i<j<l$, $g(ij)$ means $f^{*}(i'j')\,f(ij)$ and if $i<l<j$, $g(ij)$ means $f^{*}(i'j)\,f(ij)$. Under the assumption of short range forces the quantities $h(ij)$ tend rapidly to zero with increasing $r_{ij}$.

Writing

$$F^{*} F = Q(A) = \prod_{i<j\leqslant n} g(ij) \prod_{\substack{k\leqslant n\\ l>n}} (1+h(kl))\,Q(A-n) \tag{12}$$

and expanding $\prod(1+h(kl))Q(A-n)$ we get an expansion of the form

$$Q(A) = \sum_{\lambda} \frac{(A-n)!}{(A-n-\lambda)!}\, G_{\lambda}^{(n)}(1 \dots n+\lambda)\, Q(A-n-\lambda), \tag{13}$$

where

$$G^{(n)}(1 \dots n+\lambda) = G_0^{(n)}(1 \dots n)\,\frac{1}{\lambda!}\sum \prod h(ij) \tag{13'}$$

with

$$G_0^{(n)}(1 \dots n) = \prod_{i<j\leqslant n} g(ij) \quad n>1$$

and

$$G_0^{(1)}(1 \dots n) = 1.$$

The symbolic sum of products in (13′) can as in gas theory be represented by diagrams where each factor $h(ij)$ is represented by a line connecting the two points $i$ and $j$. The expansion (13) is such that each part of a diagram must have at least one connexion with the basis set $1\dots n$. Except for the fact that no simplifications appropriate for a uniform gas must be introduced here, the procedure is the same as that described by Mayer and Montroll [7] for a classical gas and we refer to their paper for further details.

Introducing the expansion (13) into (10) we get

$$(1'2'\dots n'|\varrho|12\dots n)=\sum_{\lambda}\frac{A!}{(A-n)!}\times$$

$$\times\frac{\int G_{\lambda}^{(n)}(1\dots n+\lambda)\,Q(A-n-\lambda)\langle 1'\dots n', n+1\dots A|\varrho|1\dots n, n+1\dots A\rangle\, d\tau^{A-n}}{\int Q(A)\langle 1\dots A|\varrho|1\dots A\rangle\, d\tau^{A}}. \tag{14}$$

Because of the effect of exchange between the particles $1\dots n+\lambda$ and the remaining particles, we cannot factorize (14) directly as in classical theory. Instead we can proceed as follows by successive expansions. For the sake of brevity we first introduce the shorter notations

$$\varrho_n=(1'\dots n'|\varrho|1\dots n) \quad\text{and}\quad \varrho_n^D=\langle 1'\dots n'|\varrho|1\dots n\rangle.$$

I. In the first step we make use of the Laplace expansion of a determinant, which applied to $\varrho_A^D=\det_A\langle x_i'|\varrho|x_i\rangle$ gives

$$\varrho_A^D=\varrho_{n+\lambda}^D\,\varrho_{A-n-\lambda}^D+R_{n\lambda}, \tag{15}$$

where $R_{n\lambda}$ is the sum of all the terms representing exchanges between the particles $1\dots n+\lambda$ and the remaining ones. The first term permits a factorisation and gives the contribution

$$\sum_{\lambda}Z(n+\lambda)\int G_{\lambda}^{(n)}(1\dots n+\lambda)\,\varrho_{n+\lambda}^D\,d\tau^{\lambda} \tag{16}$$

with

$$Z(m)=\frac{A!}{(A-m)!}\,\frac{\int Q(A-m)\,\varrho_{A-m}^D\,d\tau^{A-m}}{\int Q(A)\,\varrho_A^D\,d\tau^{A}}. \tag{16′}$$

We note that if we expand $Q(A)$ in the denominator in (16′) and apply (15) with neglect of $R_{n\lambda}$ we get for $n=2$ a trivial generalisation of Jastrow's derivation of the pair distribution function. In this approximation all exchanges between the particles $1\dots n+\lambda$ are taken into account, but the exchanges with the remaining particles are neglected. These exchanges give exchange couplings between clusters, which are disconnected in classical theory. Such effects are taken into account by Iwamoto and Yamada [2] and have recently been discussed by Hartogh and Tolhoek [4]. The exchange effects are contained in the terms $R_{n\lambda}$ in (15). The Laplace expansion is of no direct use as $Q(A-n-\lambda)$ contains all kinds of clustering between the particles, so we use instead the following procedure.

II. We wish first to consider exchanges between two groups of connected particles only. We then consider an expansion of a similar form as (13) but with $G_\lambda^{(n)}(1\ldots n+\lambda)$ replaced by the product of two functions, one containing all the connexions with the basis and having the same structure as $G_\lambda^{(n)}$ itself, the other having no connexions with the basis and being such that each diagram is connected, i.e. we can go from any of its lines to any other by continuous displacement on the diagram. One finds easily that this corresponds to replacing $Q(A-n-\lambda)$ in (13) by

$$\sum_{\mu=1}\frac{(A-n-\lambda)!}{(A-n-\lambda-\mu)!}G_\mu^{(0)}(n+\lambda+1\ldots n+\lambda+\mu)\,Q(A-n-\lambda-\mu) \tag{17}$$

the index 0 indicating that there is no connexion with the basis $1\ldots n$. We wish to consider exchanges between the particles $1\ldots n+\lambda$ and $n+\lambda+1\ldots n+\lambda+\mu$ only. Then applying the Laplace expansion as in I we can for each $\lambda$ separate the integral over the factor $Q(A-n-\lambda-\mu)$. We have then, however, included also terms which only give interchanges within the two sets of coordinates. Those terms are easily eliminated by replacing $\varrho^D_{n+\lambda+\mu}$ by

$$[\varrho]_{n\lambda\mu}=\varrho^D_{n+\lambda+\mu}-\varrho^D_{n+\lambda}\varrho^D_\mu. \tag{18}$$

For each $\lambda$ we then get the contribution

$$\sum_{\mu=1}Z(n+\lambda+\mu)\int G_\lambda^{(n)}(1\ldots n+\lambda)\,G_\mu^{(0)}(n+\lambda+1\ldots n+\lambda+\mu)\,[\varrho]_{n+\lambda+\mu}\,d\tau^{\lambda+\mu}. \tag{19}$$

III. These arguments can now be repeated to include exchange coupling between an arbitrary number of disconnected sets of particles. To consider exchange coupling between three disconnected sets we replace for each $\lambda$ and $\mu$ $Q(A-n-\lambda-\mu)$ in (17) by

$$\sum_{\nu=1}\frac{(A-n-\lambda-\mu)!}{(A-n-\lambda-\mu-\nu)!}G_\nu^{(0)}(n+\lambda+\mu+1\ldots n+\lambda+\mu+\nu)\,Q(A-n-\lambda-\mu-\nu). \tag{20}$$

Factorising the expression as in II we get for each $\lambda$ and $\mu$ the three-clusters exchange contributions expressed as

$$\begin{aligned}\sum_{\nu=1}Z(n+\lambda+\mu+\nu)\int G_\lambda^{(n)}(1\ldots n+\lambda)\,G_\mu^{(0)}(n+\lambda+1\ldots n+\lambda+\mu)\times\\ \times G_\nu^{(0)}(n+\lambda+\mu+1\ldots n+\lambda+\mu+\nu)\,[\varrho]_{n+\lambda+\mu+\nu}\,d\tau^{\lambda+\mu+\nu}.\end{aligned} \tag{21}$$

Here $[\varrho]_{n+\lambda+\mu+\nu}$ is determined so that in each diagram the three sets become connected if we represent each exchange by a certain type of link [4]. The expression for $[\varrho]_{n+\lambda+\mu+\nu}$ is easily written down by subtracting from $\varrho_{n+\lambda+\mu+\nu}$ those components which correspond to forbidden diagrams. Denoting the three sets by 1, 2 and 3 for simplicity, we get the following forbidden diagrams.

1) 1, 2 and 3 all disconnected, which corresponds to $\varrho_1^D\varrho_2^D\varrho_3^D$ (no exchange between the groups).
2) Two sets (e.g. 1 and 2) connected by exchange, and the third (3) disconnected, which corresponds to $\varrho_3[\varrho_{1+2}-\varrho_1\varrho_2]$ and correspondingly for the other two cases.

We then get

$$[\varrho]_{1+2+3} = \varrho^D_{1+2+3} - \varrho^D_1 [\varrho^D_{2+3} - \varrho^D_2 \varrho^D_3] - \varrho^D_2 [\varrho^D_{1+3} - \varrho^D_1 \varrho_3] - \varrho^D_3 (\varrho^D_{1+2} - \varrho^D_1 \varrho^D_2) - \varrho^D_1 \varrho^D_2 \varrho^D_3 .$$

Proceeding in this way we end up with an expansion of the form

$$\begin{aligned}\varrho_n = {} & Z(n)\, G_0^{(n)}(1 \dots n)\, \varrho_n + \sum_{\lambda=1} Z(n+\lambda) \int G_\lambda^{(0)}(1 \dots n+\lambda)\, \varrho^D_{n+\lambda}\, d\tau^\lambda + \\ & + \sum_{\lambda=0} \sum_{\mu=1} Z(n+\lambda+\mu) \int G_\lambda^{(n)}(1 \dots n+\lambda)\, G_\mu^{(0)}(n+\lambda+1 \dots n+\lambda+\mu)\, [\varrho]_{n+\lambda+\mu}\, d\tau^{\lambda+\mu} + \\ & + \sum_{\lambda=0} \sum_{\mu=1} \sum_{\nu=1} Z(n+\lambda+\mu+\nu) \int G_\lambda^{(n)}(1 \dots n+\lambda)\, G_\mu^{(0)}(n+\lambda+1 \dots n+\lambda+\mu) \times \\ & \times G_\nu^{(0)}(n+\lambda+\mu+1 \dots n+\lambda+\mu+\nu)\, [\varrho]_{n+\lambda+\mu+\nu}\, d\tau^{\lambda+\mu+\nu} + \cdots \end{aligned} \tag{22}$$

This formula can now be simplified essentially by taking together certain classes of terms. We note that in deriving (22) we make use of formulas like (17) and (19) where the terms $\mu = 1$, $\nu = 1, \dots$ represent a cluster consisting of one single point. Such terms in (22) which contain single points can be reduced noting that the integrands contain factors of the type

$$\langle x_i | \varrho | x_\sigma \rangle \langle x_\sigma | \varrho | x_j \rangle,$$

$x_\sigma$ being the coordinate for an isolated point. As the integrand does not depend on $x_\sigma$ in any other way, the integration over $x_\sigma$ gives the result

$$\langle x_i | \varrho | x_j \rangle$$

which means that the integral reduces to one where this particular one-particle cluster does not appear. In this way every integral with a number of single-point clusters can be reduced (except for a numerical factor) to a term in (22) with no single-point clusters. Thus every term in (18) without any single-point clusters can be regarded as the parent of a family of terms obtained by attaching exchange links to a number of single points. The contribution from each member of the family differs only by a factor from that of the parent so the sum over the whole family will be factor times the contribution from the parent. Summing up over all such families we still have an expansion of the form (22) but with the factors $Z(m)$ replaced by new factors $Z'(m)$ and without the terms $\mu = 1$, $\nu = 1 \dots$

$$\begin{aligned}\varrho_n = {} & Z'(n)\, G_0^{(n)}(1 \dots n)\, \varrho^D_n + \sum_{\lambda=1} Z'(n+\lambda) \int G_\lambda^{(n)}(1 \dots u+\lambda)\, \varrho^D_{n+\lambda}\, d\tau^\lambda + \\ & + \sum_{\lambda=0} \sum_{\mu=2} Z'(n+\lambda+\mu) \int G_\lambda^{(n)}(1 \dots n+\lambda)\, G_\mu^{(0)}(n+\lambda+1 \dots n+\lambda+\mu)\, [\varrho]_{n+\lambda+\mu}\, d\tau^{\lambda+\mu} + \\ & + \sum_{\lambda=0} \sum_{\mu=2} \sum_{\nu=2} Z'(n+\lambda+\mu+\nu) \int G_\lambda^{(n)}(1 \dots n+\lambda)\, G_\mu^{(0)}(n+\lambda+1 \dots n+\lambda+\mu) \times \\ & \times G_\nu^{(0)}(n+\lambda+\mu+1 \dots n+\lambda+\mu+\nu)\, [\varrho]_{n+\lambda+\mu+\nu}\, d\tau^{\lambda+\mu+\nu} + \cdots \end{aligned} \tag{23}$$

The new normalisation constants $Z'(m)$ are obviously given as a linear combination of the constants $Z(n)$ for $n \geqslant m$. Expanding the integrand in the denominator in (16′) in the same way as in our treatment of the numerator in (10) one finds, if neglecting terms which tend to zero when $A$ goes to infinity, that $Z'(m)$ satisfies a relation of the form

$$Z'(m) = \left[1 + \sum_{i=1} \alpha_i^{(m)} \frac{Z'(m+i)}{Z'(m)}\right]^{-1}. \tag{24}$$

The constants $\alpha_i^{(m)}$ depend on the strength of the two-body correlation through a parameter, which for a uniform gas is simply $\eta = A w_c / \Omega$, where $w_c$ is the weighted volume in which the correlation is appreciable and $\Omega$ is the volume. $\alpha_i^{(m)}$ tend to zero when $\eta$ goes to zero. Further for $m \ll A$ it is easily found that

$$\frac{Z'(m+1)}{Z'(m)} = Z' \quad \text{(independent of } m\text{)}. \tag{24'}$$

Assuming that the expansions converge rapidly enough only terms fulfilling this condition will be of importance and then only powers of $Z'$ will appear in (23).

The formulas given above are obtained by first taking the single-point clusters into account and then reducing the formulas. If we simply had left out these single-point clusters from the beginning, we would have obtained (23) but with the original normalisation constants $Z(m)$ instead of $Z'(m)$. It is now simple to show that if we treat the denominator in (16′) in the same way, i.e. neglect all single points in the expansion of $Q(A)$, the original $Z(m)$ satisfies the relation (24) with the same $\alpha_i^{(m)}$ and further that $Z(m+1)/Z(m) = Z$ (independent of $m$). From this we can conclude that $Z' = Z$, i.e. (23) is just the expansion we would have obtained if all exchanges involving point clusters had just been left out from the very beginning. This remark connects our approach with that by Hartogh and Tolhoek for a uniform gas, and especially we can apply their result that $Z \to 1$ as $A \to \infty$.

The final expression will thus take the form

$$\begin{aligned} \varrho_n = {} & Z^n G_0^{(n)}(1 \ldots n)\, \varrho_n^D + \sum_{\lambda=1} Z^{n+\lambda} \int G_\lambda^{(n)}(1 \ldots n+\lambda)\, \varrho_{n+\lambda}^D \, d\tau^\lambda + \\ & + \sum_{\lambda=0} \sum_{\mu=2} Z^{n+\lambda+\mu} \int G_\lambda^{(n)}(1 \ldots n+\lambda)\, G_\mu^{(0)}(n+\lambda+1 \ldots n+\lambda+\mu)\, [\varrho]_{n+\lambda+\mu}\, d\tau^{\lambda+\mu} + \\ & + \sum_{\lambda=0} \sum_{\mu=2} \sum_{\nu=2} Z^{n+\lambda+\mu+\nu} \int G_\mu^{(n)}(1 \ldots n+\lambda)\, G_\mu^{(0)}(n+\lambda+1 \ldots n+\lambda+\mu) \times \\ & \times G_\nu^{(0)}(n+\lambda+\mu+1 \ldots n+\lambda+\mu+\nu)\, [\varrho]_{n+\lambda+\mu+\nu}\, d\tau^{\lambda+\mu+\nu} + \cdots \end{aligned} \tag{25}$$

It is now a trivial matter to write down the first few terms in the expansions of $\varrho_1$ and $\varrho_2$, from which one then gets the expansion of the energy. We do not give those rather lengthy formulas here, as we have here wished to indicate this method of deriving the expansion only, rather than give all the details. More of the details will be given in a forthcoming paper.

Order of magnitude estimates of the terms can easily be made for a uniform system by noting that the one-particle Dirac matrix $\langle x' | \varrho | x \rangle$ is a smooth decreasing function of $|\boldsymbol{r}' - \boldsymbol{r}|$ proportional to $A/\Omega$ and that all exchange terms give contributions containing a lower of $A$ than the corresponding direct term, the decrease in the exponent being determined by the number of exchanges. For a non-uniform system of a reasonable structure one can also easily make order of magnitude estimates of the various terms by approximating the one-particle matrix locally with that for a uniform medium, i.e. consider $\langle x' | \varrho | x \rangle$ as proportional to the product of the local density times a smooth decreasing function of $|\boldsymbol{r}' - \boldsymbol{r}|$.

We note finally that the formal simplicity of this approach is effectively due to the various simple properties of the Dirac density matrices, e.g. spin and isospin do not cause any extra complications, no formal differences arise between uniform and non-uniform systems and that conservation principles associated with the particular symmetry of the system are automatically satisfied except of course for possible degeneracies.

*Institute for Theoretical Physics, University of Uppsala.*

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